Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Curl flux, coherence, and population landscape of molecular systems: Nonequilibrium quantum steady state, energy (charge) transport, and thermodynamics ZHEDONG ZHANG, JIN WANG, SUNY Stony Brook — We established a theoretical framework in terms of the curl flux, population landscape, and coherence for non-equilibrium quantum systems at steady state, through exploring the energy and charge transport in molecular processes. The curl quantum flux plays the key role in determining transport properties and the system reaches equilibrium when flux vanishes. The novel curl quantum flux reflects the degree of non-equilibriumness and the time-irreversibility. We found an analytical expression for the quantum flux and its relationship to the environmental pumping (non-equilibriumness quantified by the voltage away from the equilibrium) and the quantum tunneling. Furthermore, we investigated another quantum signature, the coherence, quantitatively measured by the non-zero off diagonal element of the density matrix.quantum flux is promoted by the coherence in the regime of small tunneling while reduced by the coherence in the regime of large tunneling, due to the non-monotonic relationship between the coherence and tunneling. For the systems coupled to bosonic (photonic and phononic) reservoirs the flux is significantly promoted at large voltage while for fermionic (electronic) reservoirs the flux reaches a saturation after a significant enhancement at large voltage.

Zhedong Zhang
SUNY Stony Brook

Date submitted: 14 Nov 2014 Electronic form version 1.4